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## Reactivity of Paramagnetic Fe-II-Bis(amidinate) Complexes

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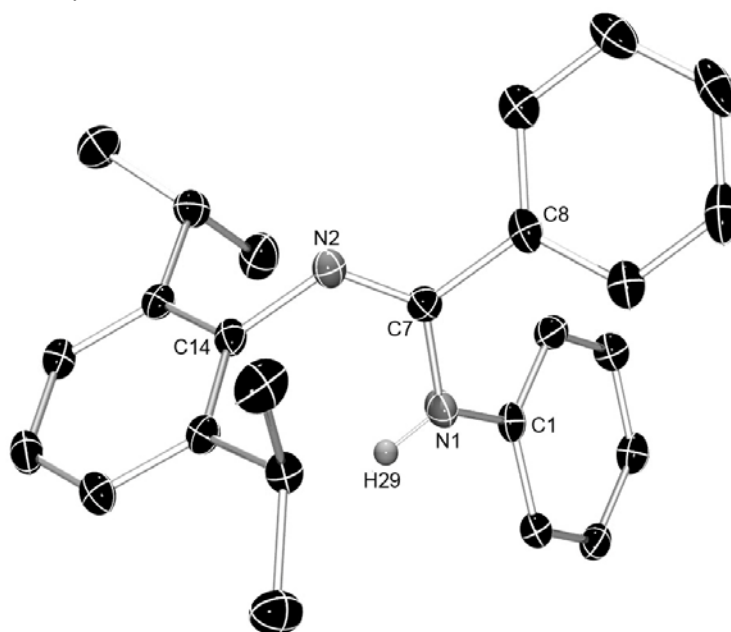
**SUPPORTING INFORMATION**

**DOI:** 10.1002/ejic.201000717

**Title:** Reactivity of Paramagnetic Fe<sup>II</sup>–Bis(amidinate) Complexes

**Author(s):** Erica Jellema, Timo J. J. Sciarone,\* Noa M. Navarrete, Marten J. Hettinga, Auke Meetsma, Bart Hessen

X-ray structure of <sup>DippPh</sup>LH:



**Figure S1.** Molecular structure of <sup>DippPh</sup>LH (50% probability level). Hydrogen atoms (except NH) removed for clarity.

**Table S1.** Selected bond distances and angles for <sup>DippPh</sup>LH.

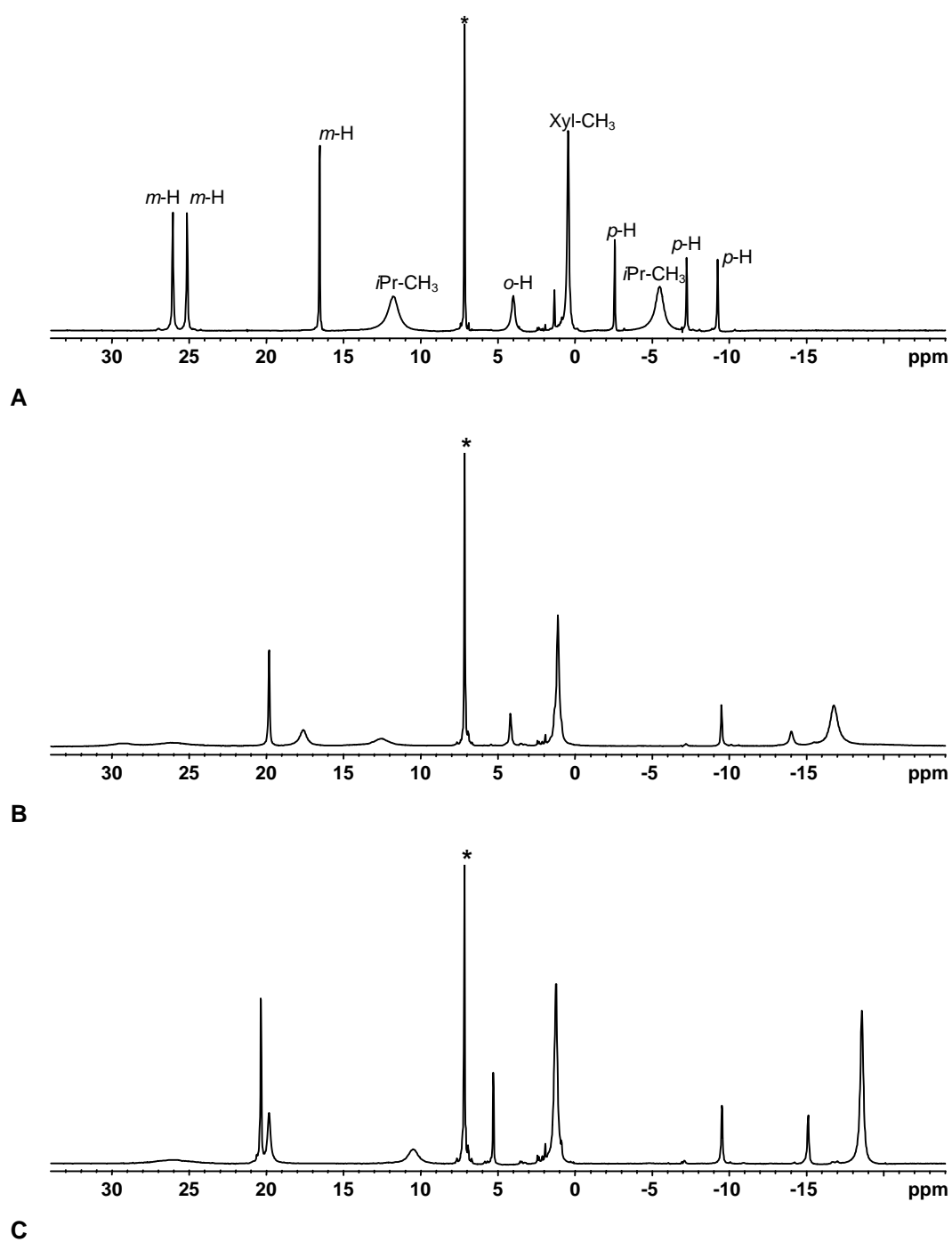
Distances [Å]			
N1-C1	1.416(3)	N2-C14	1.425(3)
N1-C7	1.392(3)	C7-C8	1.494(3)
N2-C7	1.281(3)	N1-H29	0.84(2)
Angles [°]			
C1-N1-C7	125.36(18)	N1-C7-N2	124.6(2)
C7-N1-H29	112.3(15)	N1-C7-C8	117.45(18)
C1-N1-H29	117.3(16)	N2-C7-C8	117.64(19)
C7-N2-C14	121.64(17)		

**Table S2.** Crystal, collection and refinement data for <sup>DippPh</sup>LH.

formula	C <sub>25</sub> H <sub>28</sub> N <sub>2</sub>	$\rho_{\text{calc}}$ (g/cm <sup>3</sup> )	1.168
fw	356.49	$\theta$ range (°)	2.68 – 27.39
cryst. dim. (mm)	0.34 x 0.22 x 0.13	$\lambda$ (Å)	0.71073 (Mo K $\alpha$ )
colour, habit	l. yellow, block	$T$ (K)	100(1)
crystal system	monoclinic	data collect. time (h)	5.6
space group, no. <sup>53</sup>	$P2_1/c$ , 14	no. of meas. refl.	7492
$a$ (Å)	8.2831(7)	no. of unique refl.	4050
$b$ (Å)	23.574(2)	$\mu$ (cm <sup>-1</sup> )	0.68
$c$ (Å)	10.735(1)	no. of parameters	356
$\alpha$ (°)	90	weighting scheme: a,b <sup>[a]</sup>	0.0821, 0.0
$\beta$ (°)	104.647(2)	$R(F)$ for $F_0 \geq 4\sigma(F_0)$ <sup>[b]</sup>	0.0557
$\gamma$ (°)	90	$wR(F^2)$ <sup>[c]</sup>	0.1593
$Z$	4	res. el. dens. (e/Å <sup>3</sup> )	-0.28, 0.36(6)
$V$ (Å <sup>3</sup> )	2028.1(3)	GoF <sup>[d]</sup>	1.044

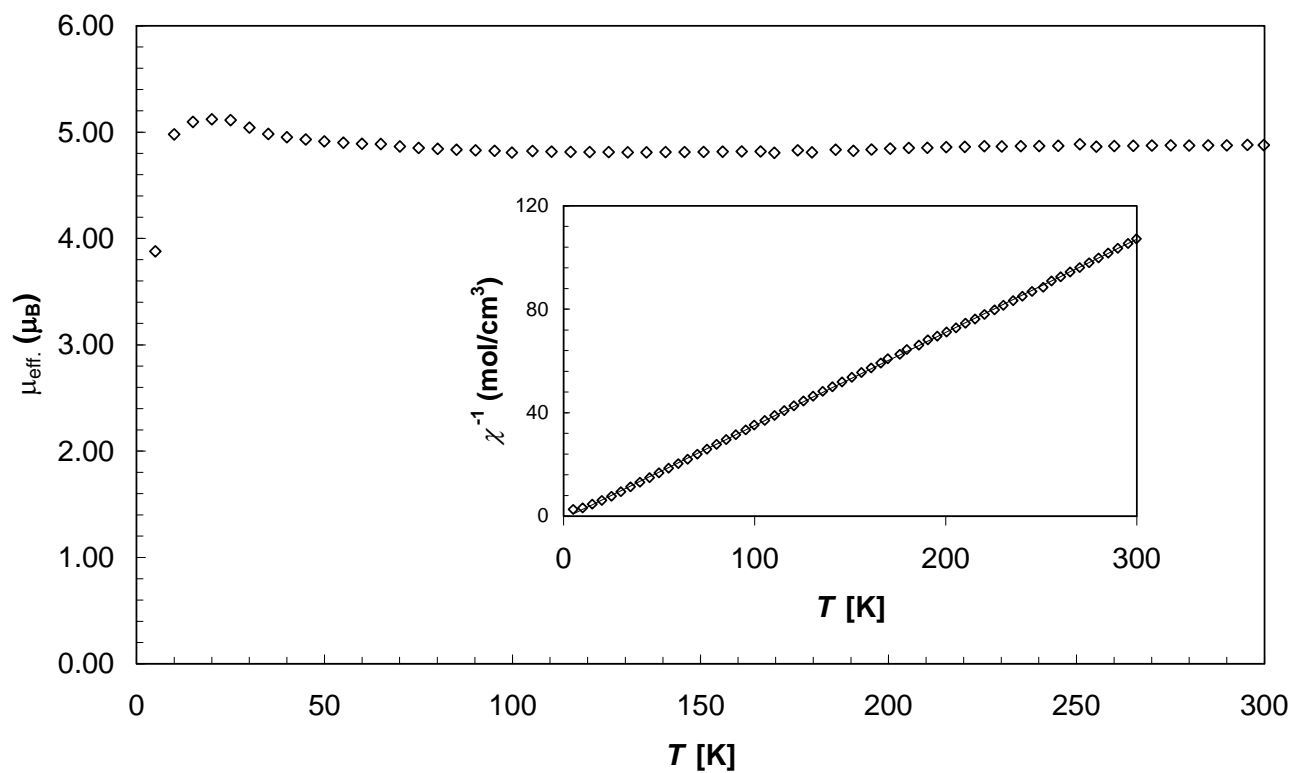
<sup>[a]</sup>  $w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP]$ ,  $P = [\max(F_o^2, 0) + 2F_c^2] / 3$  <sup>[b]</sup>  $R(F) = \sum (|F_o| - |F_c|) / \sum |F_o|$  <sup>[c]</sup>  $wR(F^2) = [\sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2]]^{1/2}$  <sup>[d]</sup>  $\text{GoF} = [\sum [w(F_o^2 - F_c^2)^2] / (n-p)]^{1/2}$ , n = # refl., p = # param. refined.

Reactions of **1b** with pyridine:



**Figure S3.**  $^1\text{H}$  NMR spectra (300 MHz,  $\text{C}_6\text{D}_6$ , 298 K) of **1b** (A), **1b** + 1 equiv. py (B) and **1b** + 2 equiv. py (C)

Magnetic Susceptibility for **1c.bpy**.



**Figure S4.**  $\mu_{\text{eff}}$  and  $\chi^{-1}$  for vs  $T$  for **1c.bpy**.